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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for Calculations of Salado Flow: Technical Baseline Migration (TBM)

AP-086

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1 INTRODUCTION AND OBJECTIVES

The Technical Baseline Migration (TBM) (Lord and Hadgu, 2002a; Wall, 2001) will merge parameters defined in the Compliance Certification Application (CCA) with those defined by the Performance Assessment Verification Test (PAVT) (PAVT, 1997; EPA, 1998) in order to establish a single performance assessment technical baseline for the Waste Isolation Pilot Plant (WIPP). In addition, the TBM offers an opportunity for DOE to implement several important changes to the conceptual models used by WIPP Performance Assessment (PA).

This analysis plan describes 1) the conceptual model changes related to flow in the Salado Formation and 2) the set of calculations of Salado flow that are planned for the TBM PA. All conceptual model changes will be presented to a peer review panel in accordance with regulatory procedures.

2 CONCEPTUAL MODEL CHANGES: FLOW IN THE SALADO

Primarily, there are two conceptual models that will be affected by the planned TBM calculations. All conceptual model changes will be presented to a peer review panel with detailed explanations and justifications. Listed below is a brief outline of the changes that directly affect the Salado flow calculations planned for the TBM.

2.1 Disposal System Geometry

This conceptual model (CM) describes how the various components of the repository (waste panels, panel closures, shaft seals, operations and experimental areas) are represented in the BRAGFLO grid. Specifically, this CM defines parameters such as length, height, volume, and position of these components, and describes how they are represented in the finite difference grid. This CM assumes that the spatial effects of process interactions that will occur in and around the repository can be represented by a two dimensional grid oriented as a vertical cross-section with “radial flaring”. This conceptual model acknowledges that while actual flow will not be truly radial, the two-dimensional flared grid is sufficient for estimating calculated releases. The CCA BRAGFLO grid has several scales of “radial flaring,” including local-scale flaring around the intrusion borehole and shaft and regional-scale flaring away from the repository. The flaring is implemented by calculating the grid cell thickness in the Z dimension (ΔZ) for each grid cell increment in the X dimension (ΔX)[1]. For the CCA the ΔZ for each grid column was calculated by a series of complicated cell wrapping procedures. The CCA method is very difficult to reproduce and makes subsequent changes difficult to implement.

1 The grid is 2-D in the X-Y plane (Figure 2), but each cell has a “thickness” in the Z-dimension, ΔZ. The ΔZ values are the same for all cells in a column.

For the TBM, we propose to make several changes to this conceptual model. First, since the performance of the shaft seal system has been shown by modeling to be exceedingly effective in preventing flow up the shaft, we propose to remove this component from the model domain. Because the shaft in the CCA grid was a center for local grid flaring, its removal required recalculating the flaring for the whole grid. Since the flaring is a function of all the grid cell dimensions and positions in the X-direction, removal of the shaft presented the opportunity to make two additional changes that also affect the X-dimensions of grid cells (more detail in the panel closures and rest of repository, as described below). The second change implements a robust panel closure that is designed to prevent flow between panels during the regulatory period (Figure 1). For the CCA, the Department of Energy (DOE) presented four options for panel closure designs (A-D). The Environmental Protection Agency (EPA) as a condition for certification mandated the implementation of Option D, which is designed to provide the tightest closure between panels. For the TBM we plan to implement the cross-sectional area of the panel closures consistent with the plans for Option D and enhance detail of the modeled WIPP underground relative to the CCA. It is important to acknowledge that while the dimensions of the modeled panel closures closely match the Option D design, the model domain is too coarse to adequately evaluate specific design features. Rather, these PA calculations can evaluate the possible futures of repository performance assuming that panel closures act as effective hydrologic barriers during the regulatory period.

The third change divides the CCA "rest of repository" block into two blocks separated by a panel closure.

The fourth change simplifies the way ΔZ and the regional-scale flaring is calculated so that the grid is easily reproducible and can accommodate changes in the future. The new flaring algorithm (Stein and Hadgu, 2002) calculates the ΔZ for cells to the north and south of the excavated area only. It assumes that the center from which the flaring should be calculated lies at the center of mass of the waste filled regions rather than using two centers (at the borehole and the shaft) as was done for the CCA grid. The ΔZ can be calculated using a formula that assumes simple repository geometry. The new method calculates flaring that is nearly identical to the CCA grid and allows future changes to be made to the ΔX dimensions of grid cells. We propose to use the flaring algorithm to add more grid cells in the X-direction to the north and south of the repository to improve the numerical performance of the model.

A fifth change vertically refines the grid above and below Marker Bed 139. This marker bed is 0.85 m-thick but was surrounded by layers that were 11 and 1.38 m-thick in the CCA grid. We propose to add two additional layers that are ≤ 1.0 m-thick. This change will decrease numerical dispersion observed in this layer during the CCA and PAVT.

The logical grid to be used for the TBM PA is shown in Figure 2.

2.2 Disturbed Rock Zone

This conceptual model describes the hydraulic and physical parameters used to represent the Disturbed Rock Zone (DRZ). The most important of these parameters are permeability and porosity. For the CCA, DRZ permeability was held constant at 10^{-15} m^2. For the PAVT, the permeability was sampled from $10^{-19.4}$ to $10^{-12.5}$ m^2 with a median permeability of $10^{-15.95}$ m^2. In addition, the pressure-induced fracture model (designed for the anhydrite marker beds) was applied to the DRZ in order that the vectors with very low DRZ permeability would not reach unrealistic pressures.

For the TBM, we propose using the PAVT distribution of permeability for the whole DRZ but applying the pressure dependent fracture model only to the DRZ *below* the repository. This application of the fracture model to the lower DRZ is reasonable as a simulation of the expectation that if pressures are high enough, fluids will circumvent the concrete monolith by flow in the direction normal to the plane of the grid through fractures in MB 139. These fractures are expected because of the effects of floor heave prior to emplacement of the monolith, and because of the ability of MB 139 to hydrofracture as pressures approach and exceed lithostatic levels in the real repository. In addition, the permeability of cells immediately above the concrete part of the panel closures in the upper DRZ will be sampled to reflect the range expected for healed DRZ. This change is meant to capture the effect of rigid panel closures that include excavation of the DRZ immediately surrounding the concrete monolith that is emplaced quickly to prevent the further local development of DRZ, and healing of the DRZ due to compressive stresses imposed by creep closure around the rigid structure. In this way the panel closures are modeled as effective seals, including healing effects, in accordance with their design.

3 BRAGFLO CODE CHANGES

BRAGFLO version 4.10 has been modified to change the molecular weight of cellulose and the PARAMS.INC file has been modified to accommodate the increased size of the grid. The new version is 4.10.02. Additional changes that affect direct brine release calculations are discussed in another analysis plan (Lord and Hadgu, 2002b).

3.1 Molecular Weight of Cellulose

For the CCA and PAVT, the molecular weight of cellulosics used by BRAGFLO assumed a molecular formula in the form CH_2O. This representation was inconsistent with other models used in the PA that assumed the molecular formula to be $C_6H_{10}O_5$. The following changes were made to BRAGFLO to represent cellulosics as $C_6H_{10}O_5$ and correct the previous error in implementation.

- Comments were put in BRAGFLO MAIN to identify the changes made.

- Molecular weight of cellulose was changed from 30.02628 x 10^{-3} to 27.023 x 10^{-3} kg/mol (value is actually molecular weight normalized for a single carbon {equals molecular weight of $CH_{10/6}O_{5/6}$})
- Any references to CH_2O were replaced by $C_6H_{10}O_5$.
- Any variable names with CH2O were replaced.

4 PARAMETER CHANGES FOR THE TBM

In support of the implementation of the Option D-type panel closure outlined in section 2.1 of this Analysis Plan we will introduce two new materials and associated properties. The non-concrete portion of the PCS, including the explosion wall and the gap between this and the concrete monolith, will be assigned the material WAS_AREA with a permeability of ~2.4 x 10^{-13}. The new materials are described below.

4.1 *Panel Closure Concrete (CONC_PCS)*

The EPA required Option D and the use of Salado Mass Concrete (SMC) as conditions of their rule (Appendix A to Part 194 Condition 1). The EPA required use of salt-saturated concrete as designed for the shaft seal system. Design of the shaft seal system included justification of material properties, including permeability (SAND96-1326).

One of the assumptions employed in the CCA was that cementitious materials would degrade after 400 years. However, a subsequent and more detailed evaluation (Thompson and Hansen, 1996) concluded that no significant degradation is expected for the concrete members of the panel closure concrete. They show that potential flow through the concrete closure is nearly two orders of magnitude too small to cause any significant degradation.

Material parameters for shaft seal system elements are summarized in Hurtado et al. (1997). The permeability of the SMC seal components was treated as a random variable defined by a log triangular distribution with a best estimator of 1.78 x 10^{-19} m^2 and lower and upper limits of 2.0 x 10^{-21} and 1.0 x 10^{-17} m^2, respectively. The selected permeability range for SMC panel closure concrete in this analysis plan will use this same distribution.

For the concrete that is at the same elevation as MB 139 we will apply the anhydrite fracture model. This application does *not* imply that we expect this material to fracture directly. We allow these cells to fracture to simulate the expectation that if pressures are high enough, fluids will circumvent the concrete monolith by flow in the direction normal to the plane of the grid through fractures in MB 139. These fractures are expected because of the effects of floor heave prior to emplacement of the monolith, and because of the ability of MB 139 to hydrofracture as pressures approach and exceed lithostatic levels in the real repository. These hydrofractures have been shown to occur in MB 139 under high pressures (Wawersik, et al., 1997). While we cannot model such flows directly with a 2-D grid, by allowing the concrete cells to fracture in the model we simulate the effect of this process of flow *around* the panel closures in the case that MB 139 hydrofractures.

4.2 DRZ above Panel Closure (DRZ_PCS)

Option D panel closures are designed to remove the DRZ above and below the panel entry drifts. The depth of cut below the floor would remove the anhydrite MB 139. Loose salt in the roof would also be taken down just prior to construction of the concrete monolith. The remaining salt surrounding the panel closure concrete would be subjected to compressive stresses, which would tighten any disturbed zones. Owing to the rounded configuration of Option D, the compressive stress state creates a situation very favorable for concrete: high compressive stresses and low stress differences. In turn, the compressive stresses developed within the salt will quickly heal any damage caused by construction excavation, thereby effectively eliminating the DRZ along the length of the panel closure. The volume of salt immediately above and below the rigid concrete monolith designed as Option D would likely approach the intrinsic permeability of Salado salt.

Undisturbed Salado salt is essentially impermeable. A low-end permeability would be immeasurably low (10^{-23} m^2, for example). The salt above and below the rigid inclusion would assume relatively impermeable conditions. Permeability values employed for purposes of this Analysis Plan use the same range as described for the concrete (2×10^{-21} to 10^{-17} m^2). The reason this range was selected for this Analysis Plan rather than use the range approved for use with the intact halite is twofold. First, because the healed DRZ zone is relatively thin (7.9 m-thick in the model) small-scale heterogeneities including thin clay seams introduce uncertainties to how well this DRZ will impede flow. Second, the Panel Closure System will perform as a composite system that includes both the healed DRZ and the concrete monolith. In this system any flow will be focused through the highest permeability component of the system. In order that the PA calculations represent the uncertainties in exactly where any flow will occur during the regulatory period, we set the permeability ranges equal so that there will be an equal probability of potential flow in either material.

5 ANALYSIS OVERVIEW

Numerical model calculations similar to those conducted for the CCA and PAVT will be run to simulate flow in the Salado Formation and overlying units. The computer code BRAGFLO will be used to simulate the flow of brine and gas during the 10,000 year regulatory time period. Calculations will be performed on DEC ALPHAs (ES-40) running Open VMS Version 7.2-1. The PAVT R1 replicate (100 vectors) will be regenerated so that TBM results can be compared to PAVT results on a vector-by-vector basis. We will run three of the original six scenarios, resulting in a total of 300 BRAGFLO runs. The scenarios include (1) undisturbed {S1}, (2) E1 drilling intrusion at 1000 years after closure {S3}, and (3) E2 drilling intrusion at 1000 years after closure {S5}.

BRAGFLO input files will be generated using the suite of preprocessing codes (GENMESH, MATSET, PRELHS, LHS, POSTLHS, ICSET, ALGEBRACDB, and PREBRAG). BRAGFLO initial conditions will be calculated as in the CCA and PAVT. BRAGFLO output will be postprocessed by POSTBRAG.

For disturbed scenarios BRAGFLO and CUTTINGS_S are typically run to calculate direct releases. For the present analysis, it has not been decided whether these codes will be run. The plans for this part of the analysis are documented in Lord and Hadgu (2002b).

All code version information for the TBM is listed in Table 1.

6 SOFTWARE LIST

The software versions to be used for calculating flow and transport in the Salado formation for the TBM analysis are listed in Table 1 below.

Table 1. Software List

Code	Version
ALGEBRACDB	2.35
BRAGFLO	4.10.02
GENMESH	6.08
ICSET	2.22
LHS	2.41
MATSET	9.10
POSTBRAG	4.00
POSTLHS	4.07
PREBRAG	6.00
PRELHS	2.30

7 TASKS

Joshua Stein will handle and coordinate the development of the various model input files required to run the PA analysis through the POSTBRAG step in the calculation. Teklu Hadgu and David Lord will provide support as needed. Rodger Coman will be responsible for running the codes on the ALPHA cluster and ensuring all appropriate files are stored in the Configuration Management System (CMS).

Steve Tisinger will provide PA parameter database support. Jon Helton, Jim Garner, Joshua Stein, Teklu Hadgu, and David Lord will analyze the TBM BRAGFLO results and prepare a report to be finished by March 25, 2002. This report will be the final Sandia analysis report for this calculation set.

8 SPECIAL CONSIDERATIONS

No special considerations have been identified for this analysis.

9 APPLICABLE PROCEDURES

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

Training: Training will be performed in accordance with the requirements in NP 2-1, Qualification and Training.

Parameter Development and Database Management: Selection and documentation of parameter values will follow NP 9-2. The database is to be managed in accordance with relevant technical procedure.

Computer Codes: New or revised computer codes that will be used in the analyses will be qualified in accordance with NP 19-1. All other codes unchanged since the PAVT to be qualified under multi-use provisions of NP 19-1. The platform on which the codes will be run is the Compaq Alpha, Open VMS AXP, Version 7.2-1.

Analysis and Documentation: Documentation will meet the applicable requirements in NP 9-1.

Reviews: Reviews will be conducted and documented in accordance with NP 6-1 and NP 9-1, as appropriate.

10 REFERENCES

EPA, 1998, Technical Support Document for Section 194.23: Parameter Justification Report, U.S. Environmental Protection Agency, Office of Radiation and Indoor Air, Washington, D.C.

EPA 40CFR Part 194 Final Rule.

Hurtado, L. D., M. K. Knowles, V. A. Kelley, T. L. Jones, J. B. Ogintz, and T. W. Pfeifle. WIPP Shaft Seal System Parameters Recommended to Support Compliance Calculations, SAND97-1287, Sandia National Laboratories, Albuquerque, NM.

Lord, D.L., Hadgu, T, 2002a, Technical Baseline Migration Analysis Plan, Sandia National Laboratories, in review.

Lord, D.L., Hadgu, T, 2002b, Analysis Plan for Direct Releases as Part of the Technical Baseline Migration, Sandia National Laboratories, in review.

PAVT, 1997, Supplemental Summary of EPA-Mandated Performance Assessment Verification Test (All Replicates) and Comparison with the Compliance Certification Application Calculations, WPO # 46702, Report # 414879.

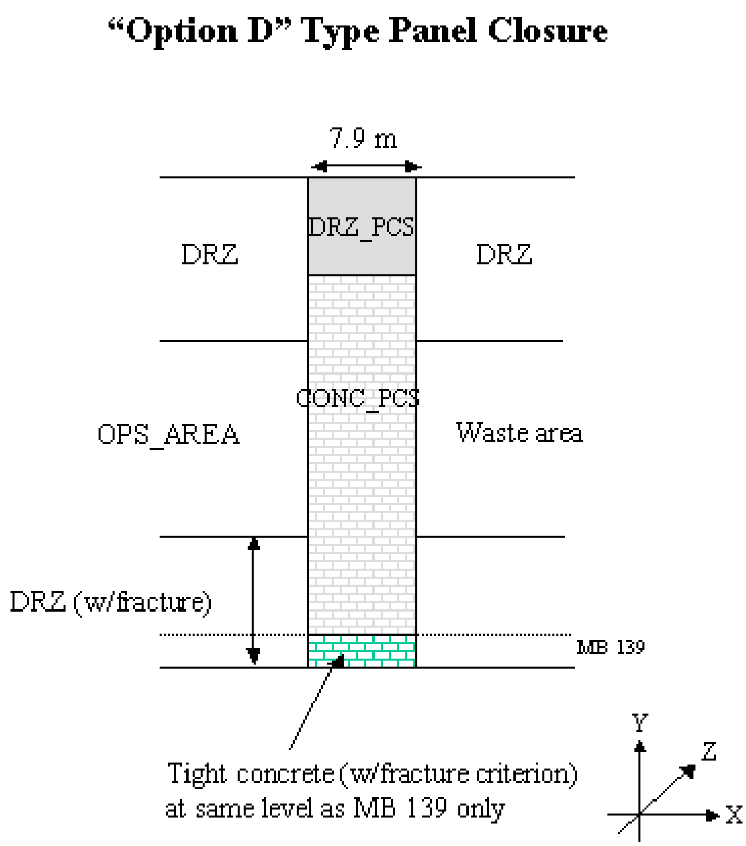
Sandia National Laboratories. 1996. Waste Isolation Pilot Plant Shaft Sealing System Compliance Submittal Design Report. Repository Isolation Systems Department 6121, SAND96-1326, Albuquerque NM.

Stein, J.S., Hadgu, T, 2002, Analysis Plan for Testing a Refined BRAGFLO Grid for the Technical Baseline Migration (TBM), AP-082.

Wall, D., 2001, Technical Baseline Migration Parameter Report, Revision 0, Sandia National Laboratories, WPO# 579510.

Wawersik, W.R., et al., Hydraulic Fracturing Tests in Anhydrite Interbeds in the WIPP, Marker Beds 139 and 140, SAND95-0596.

Figure 1. Panel closure design concept for TBM.



CONC_PCS Permeability =	2 x 10^{-21} to 10^{-17} m^2
DRZ_PCS Permeability =	2 x 10^{-21} to 10^{-17} m^2
DRZ Permeability (PAVT) =	$10^{-19.4}$ to $10^{-12.5}$ m^2
WAS_AREA Permeability =	~2.4 x 10^{-13} m^2

Figure 2. TBM BRAGFLO Grid.